IUCrData

ISSN 2414-3146

3-Methyl-2-nitroaniline

Fariha A. Bushra and Marcus R. Bond*

Department of Chemistry and Mathematics, Southeast Missouri State University, Cape Girardeau, MO 63701, USA.
*Correspondence e-mail: mbond@semo.edu

Received 3 August 2026
Accepted 14 August 2026

Edited by W. T. A. Harrison, University of Aberdeen, United Kingdom

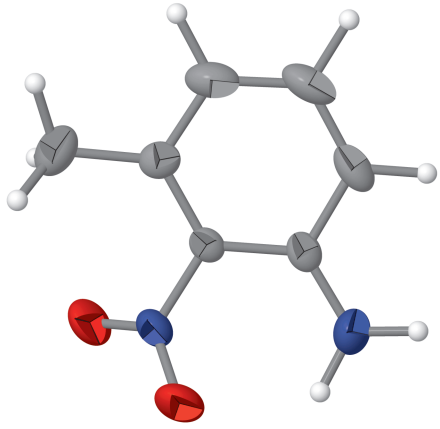
Keywords: crystal structure; supramolecular helix; aniline.

CCDC reference: 2580961

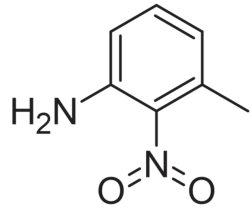
Structural data: full structural data are available from iucrdata.iucr.org

The structure of the title compound, $C_7H_8N_2O_2$, is reported and completes structural characterization for the family of methyl-2-nitroaniline isomers. Bond lengths and angles conform to reported values in other methyl-2-nitroaniline structures, except for the large angle [36.82 (4)°] formed between the phenyl ring and nitro group mean planes. This large angle is due to steric crowding by the neighboring methyl group, a result that is confirmed by an *ab initio* geometry optimization *in vacuo* that yields a similar interplanar angle (38.28°). In the extended structure, the molecules form inversion-related pairs that belong to neighboring supramolecular spiral stacks parallel to *c*. The stacks form around a 4_1 axis with N—H···N hydrogen bonding between molecules related by −1/4 of a turn at the core and peripheral N—H···O hydrogen bonds to molecules related by +3/4 of a turn.

3D view



Chemical scheme



Structure description

The title compound, $C_7H_8N_2O_2$ (**I**), is the only methyl-2-nitroaniline (M2NA) isomer with an unreported crystal structure. The geometric parameters of (**I**) (Fig. 1) conform to expected values and to the bond length and angle analysis conducted in our prior report of the structure of the 5-methyl isomer [Samson *et al.*, 2025; Cambridge Structural Database (CSD) refcode: ILADOS]. Specifically, the aniline group is almost planar [root-mean-square deviation (r.m.s.d.) = 0.056 Å from the C1/N1/H1*A*/H1*B* mean plane] with slight pyramidalization (N1 deviates by 0.097 Å from the mean plane while other atoms deviate by ∼0.03 Å on the opposite side). The nitro group is essentially planar (r.m.s.d. = 0.002 Å from the C2/N2/O1/O2 mean plane). The aniline group is nearly coplanar with the phenyl ring [dihedral angle = 4.9 (4)° between mean-plane normals] but the nitro group is not [36.82 (4)° between mean plane normals]. This large interplanar angle results from steric crowding by the neighboring methyl group – in other M2NA structures this angle is less than 6°. This result is confirmed by an *ab initio* geometry optimization [6–

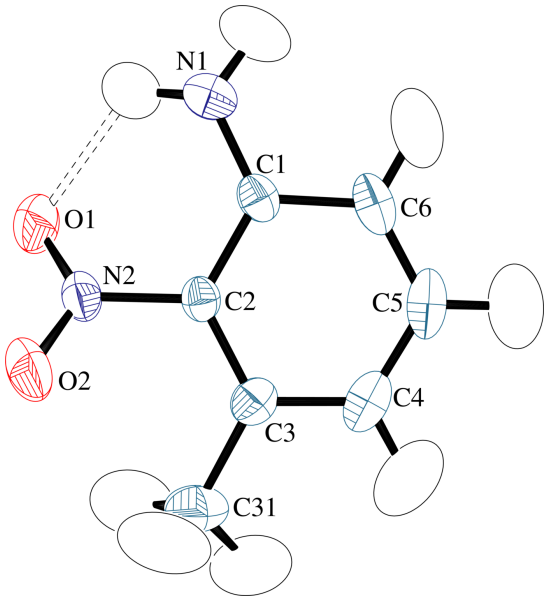


Figure 1
Displacement ellipsoid plot of (**I**) at the 50% level with labels for all non-H atoms. The intramolecular hydrogen bond is indicated by a double-dashed line.

31 G(*d*); *GAMESS* version 15 Jul 2024 (Schmidt *et al.*, 1993)] in which the value for this interplanar angle (38.26°) is in close agreement. Of note, a corresponding DFT geometry optimization [B3LYP, 6–31 G(*d*)] underestimates this angle (22.36°) but nevertheless shows the nitro group plane at a substantial twist. An electrostatic potential plot of the *ab initio* optimization is presented in Fig. 2 and the corresponding MOL file placed in supporting information.

The C—N_a (a = aniline) distance in (**I**) is significantly shorter (by 0.16 Å) than the sum of the covalent radii. This result is expected due to participation of the aniline group in the π-system of the aromatic ring and in agreement with the

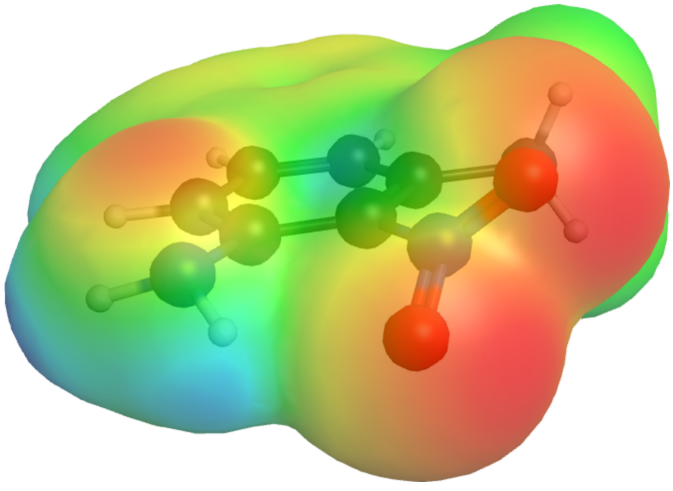


Figure 2
Electrostatic potential plot of the molecular geometry of (**I**) obtained from an *ab initio* geometry optimization. Regions of negative charge accumulation are colored red while regions of positive charge accumulation are colored blue. Atoms are drawn as spheres of arbitrary radii.

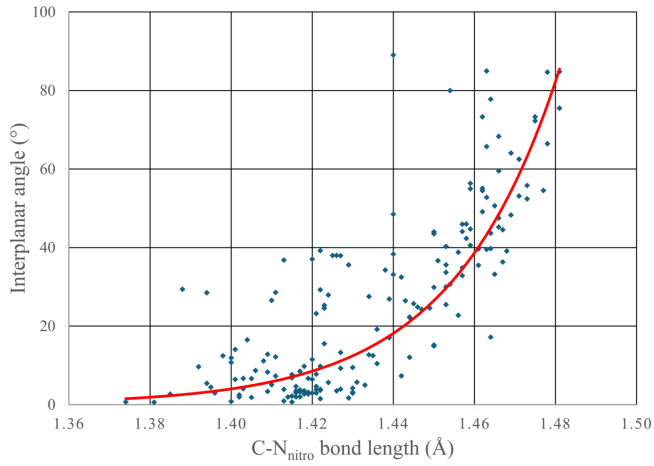


Figure 3
A plot of the angle between phenyl and nitro group mean planes (°) *versus* C—N_{nitro} bond length (Å) for 3-substituted 2-nitroaniline structures. The red curve is an empirical exponential fit.

average distance [1.349 (4) Å] in other M2NA structures. The C—N_n (n = nitro) distance is 0.07 Å less than the sum of the covalent radii and close to the average distance [1.46 (4) Å] in M2NA analogs as well as in the *ab initio* optimized geometry (1.454 Å). The large standard deviation in this average value is due to a bimodal distribution with distances of 1.50 Å in the 6-methyl analog [KEFYOK (Jing *et al.*, 2006) and KEFYOK01/02 (Callear & Hursthouse, 2009)] compared to distances in the range of 1.41–1.43 Å in the 4-methyl [TEHGUI (Ellena *et al.*, 1996); TEGHUI01 (Cannon, Glidewell, Low *et al.*, 2001); TEGHUI02 (Nigam & Murty, 1965); TEGHUI03 (Aguirre *et al.*, 2024)] and 5-methyl (ILADOS) compounds. A survey of 2-nitroaniline structures in the CSD (Version 6.01; February 2026 update; Groom *et al.*, 2016) was conducted in which substitution was required in the 3-position on the aromatic ring and possible substitution at the other positions. Values of interplanar angles between phenyl and nitro groups and C—N_n bond lengths for 91 hits were recorded and show the full range of interplanar angles. Bond lengths generally increase with interplanar angles in spite of competing effects of other ring substituents (Fig. 3). These data can be empirically fitted by an exponential function that gives an interplanar angle of ∼26° for the C—N_n bond length in (**I**). The N—O distances agree within 0.004 Å and, with an average value of 1.218 Å, are significantly shorter that the sum of the covalent radii as a result of resonance between structures with a formal single and double bond. The shorter N—O distance belongs to the O atom involved in the intramolecular hydrogen bond.

In the extended structure of (**I**), inversion-related pairs of molecules (Fig. 4), consisting of facing phenyl rings [centroid–centroid distance = 3.6498 (8) Å] slightly offset from each other [shift distance = 0.8407 (17) Å], are a readily observed structural motif. These molecules, however, belong to separate supramolecular spiral columns formed along the 4_1 screw axes (Fig. 5). Here the H atom involved in intramolecular hydrogen bonding also forms a long hydrogen bond to an aniline group on the preceding molecule related by −1/4 of a turn in the

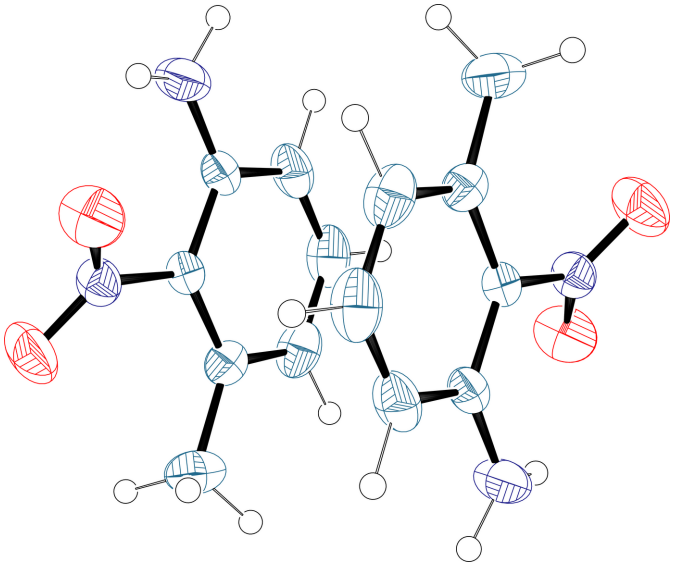


Figure 4
Displacement ellipsoid plot of an inversion-related pair of molecules in (**I**). H atoms are drawn as spheres of arbitrary radii.

spiral. The sequence of N—H···N hydrogen bonds builds the spiral structure at the core of the column (Fig. 6). A shorter N—H···O hydrogen bond to the molecule 3/4 of a turn above provides a peripheral connection that reinforces the spiral structure. Four neighboring columns aggregate about a $\overline{4}$ axis (Fig. 7). Hydrogen-bonding parameters are presented in Table 1.

The spiral columns in (**I**) are most closely related to the double spiral columns in KEFYOK/01. Here, pairs of facing, symmetrically inequivalent molecules are rotated by approximately 90° and moved up the column by a *c*-glide operation to generate an approximately square cross-section. Symmetrically inequivalent molecules related by 1/4 of a turn are connected pairwise with short N—H···O hydrogen bonds while longer N—H···O hydrogen bonds connect neighboring columns.

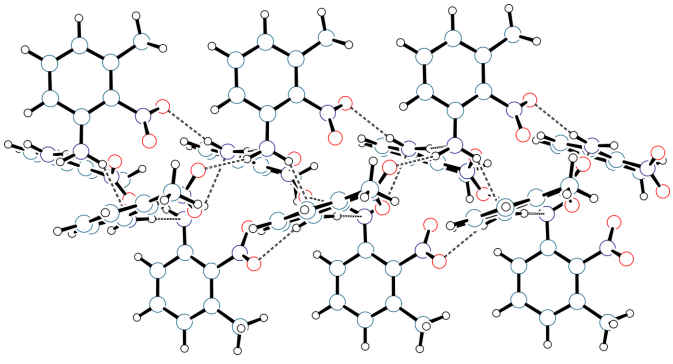


Figure 5
A plot of the supramolecular spiral structure generated by the 4_1 axis viewed with the *c* axis horizontal and [110] into the plane of the paper. Atoms are drawn as spheres of arbitrary radii and hydrogen bonds are indicated by dashed lines.

Table 1
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*B*···O1	0.987 (15)	2.052 (15)	2.7126 (15)	122.5 (11)
N1—H1*B*···N1^{i}	0.987 (15)	2.407 (15)	3.2705 (13)	145.8 (11)
N1—H1*A*···O2^{ii}	0.955 (14)	2.285 (15)	3.2108 (15)	163.0 (13)

Symmetry codes: (i) $-y+\frac{5}{4}, x-\frac{1}{4}, z-\frac{1}{4}$; (ii) $-y+\frac{5}{4}, x-\frac{1}{4}, z+\frac{3}{4}$.

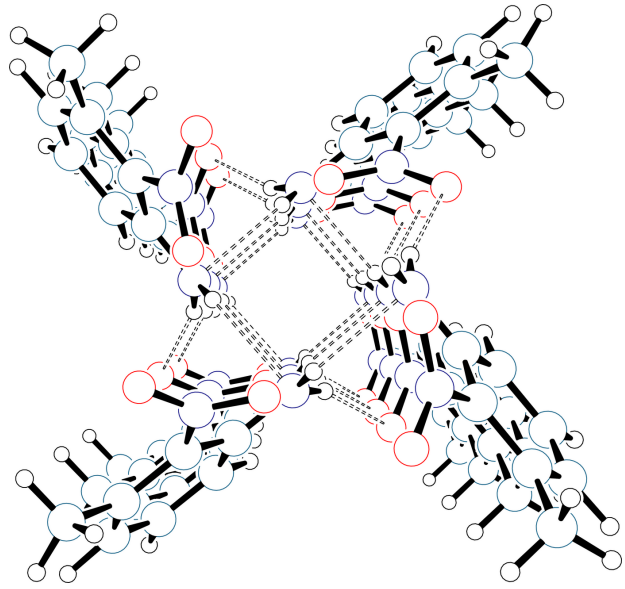


Figure 6
A plot of the molecular spiral viewed down the *c* axis with *a* horizontal and *b* vertical. Atoms are drawn as spheres of arbitrary radii and hydrogen bonds are indicated by dashed lines.

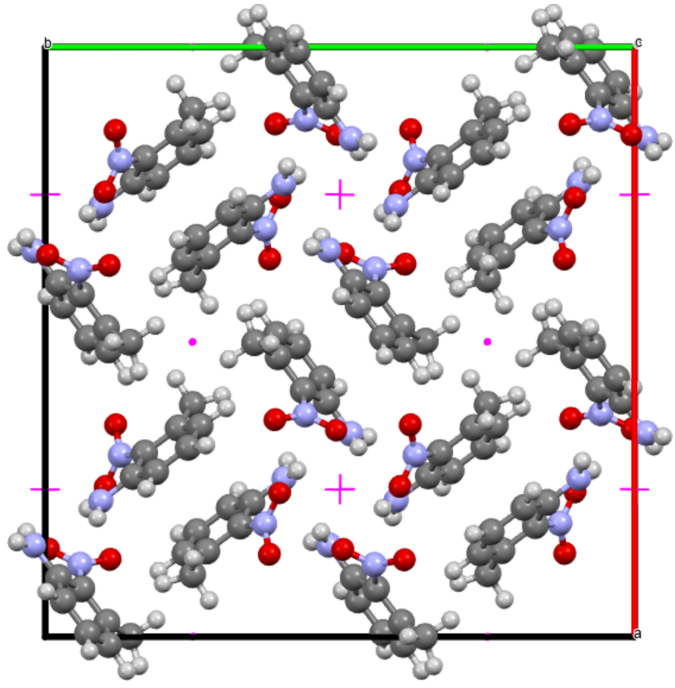


Figure 7
Packing diagram viewed down *c* with *a* vertical and *b* horizontal. 4_1 screw axes are denoted by red '+' symbols and $\overline{4}$ axes are denoted by solid red dots. Atoms are drawn as spheres of arbitrary radii.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_7H_8N_2O_2$
M_r	152.15
Crystal system, space group	Tetragonal, $I4_1/a$
Temperature (K)	295
a, c (Å)	19.8091 (6), 7.3503 (4)
V (Å^3)	2884.3 (2)
Z	16
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.11
Crystal size (mm)	0.38 × 0.36 × 0.21
Data collection	
Diffractometer	Bruker D8 Quest Eco CCD
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.910, 0.999
No. of measured, independent and observed [$I \geq 2u(I)$] reflections	85493, 2296, 1669
R_{int}	0.087
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.724
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.040, 0.075, 1.10
No. of reflections	2296
No. of parameters	172
H-atom treatment	All H-atom parameters refined
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.31, −0.31

Computer programs: *APEX3* and *SAINT* (Bruker, 2019), *SHELXT2018/2* (Sheldrick, 2015*a*), *SHELXL2018/3* (Sheldrick, 2015*b*) *OLEX2.refine* (Bourhis *et al.*, 2015), *ORTEPIII* (Burnett & Johnson, 1996), *ORTEP-3 for Windows* (Farrugia, 2012), *Mercury* 2026.1.1 (Macrae *et al.*, 2020) and *publCIF* (Westrip, 2010).

Synthesis and crystallization

3-Methyl-2-nitroaniline (99%, Ambeed) was separately dissolved in ethanol and in acetone. Orange diffraction-quality crystals were grown by slow evaporation. A crystal obtained from acetone solution provides the reported structure with no polymorphism found for crystals grown from ethanol solution. Crystals of 5-methyl-2-nitroaniline (ILADOS), previously obtained from ethanol solution, were grown from acetone solution but no polymorphic structure was found.

Refinement

Data collection and refinement parameters are presented in Table 2. Structure solution and initial refinement using an independent atom model occurred within *SHELXL2018/3* (Sheldrick, 2015*b*). Final structure refinement occurred within the *OLEX2–1.5* system *via* Hirshfeld atom refinement using *NoSpherA2* (Kleemiss *et al.*, 2021; Midgley *et al.*, 2021) with non-spherical atomic form factors derived from electron density determined by DFT calculations using *ORCA 5.0* (B3LYP functional, def2-SVP basis set; Neese, 2022). All atoms were refined anisotropically. Two low angle reflections with $F_o < F_c$ were presumed to be blocked by the beam catcher and omitted from the refinement. *APEX3* software recommended data collection to $2\theta_{max} = 66°$. However $\langle I/\sigma \rangle < 3$ for data beyond $2\theta = 62°$, so refinement was limited to $2\theta_{max} = 62°$.

Acknowledgements

Quantum mechanical calculations were conducted on the CIMUSE nodes funded by National Science Foundation grant 2322084 and incorporated as part of the Hellbender high performance computing environment at the University of Missouri-Columbia.

References

Aguirre, L. S., Litwiller, L. T., Lugo, A. N. & Thomas, A. A. (2024). *Helv. Chim. Acta* **107**, e202300244.
Bourhis, L. J., Dolomanov, O. V., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2015). *Acta Cryst.* A**71**, 59–75.
Bruker (2019). *APEX3* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Burnett, M. N. & Johnson, C. K. (1996). *ORTEPIII*. Report ORNL-6895. Oak Ridge National Laboratory, Tennessee, USA.
Callear, S. K. & Hursthouse, M. B. (2009). *Acta Cryst.* C**65**, o539–o542.
Cannon, D., Glidewell, C., Low, J. N., Quesada, A. & Wardell, J. L. (2001). *Acta Cryst.* C**57**, 216–221.
Ellena, J., Punte, G. & Rivero, B. E. (1996). *Acta Cryst.* C**52**, 2074–2076.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* B**72**, 171–179.
Jing, Z.-L., Zhang, Q.-Z., Jia, J. & Yu, M. (2006). *Acta Cryst.* E**62**, o1155–o1156.
Kleemiss, F., Dolomanov, O. V., Bodensteiner, M., Peyerimhoff, N., Midgley, L., Bourhis, L. J., Genoni, A., Malaspina, L. A., Jayatilaka, D., Spencer, J. L., White, F., Grundkötter-Stock, B., Steinhauer, S., Lentz, D., Puschmann, H. & Grabowsky, S. (2021). *Chem. Sci.* **12**, 1675–1692.
Krause, L., Herbst-Irmer, R., Sheldrick, G. M. & Stalke, D. (2015). *J. Appl. Cryst.* **48**, 3–10.
Macrae, C. F., Sovago, I., Cottrell, S. J., Galek, P. T. A., McCabe, P., Pidcock, E., Platings, M., Shields, G. P., Stevens, J. S., Towler, M. & Wood, P. A. (2020). *J. Appl. Cryst.* **53**, 226–235.
Midgley, L., Bourhis, L. J., Dolomanov, O. V., Grabowsky, S., Kleemiss, F., Puschmann, H. & Peyerimhoff, N. (2021). *Acta Cryst.* A**77**, 519–533.
Neese, F. (2022). *WIREs Comput. Mol. Sci.* **12**, e1606.
Nigam, M. & Murty, B. V. R. (1965). *Z. Kristallogr.* **122**, 318.
Samson, L., Banwart, L., Silwal, S. & Bond, M. R. (2025). *IUCrData* **10**, x250747.
Schmidt, M. W., Baldridge, K. K., Boatz, J. A., Elbert, S. T., Gordon, M. S., Jensen, J. H., Koseki, S., Matsunaga, N., Nguyen, K. A., Su, S., Windus, T. L., Dupuis, M. & Montgomery, J. A. (1993). *J. Comput. Chem.* **14**, 1347–1363.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

full crystallographic data

IUCrData (2026). **11**, x260839 [https://doi.org/10.1107/S2414314626008394]

3-Methyl-2-nitroaniline

Fariha A. Bushra and Marcus R. Bond

(I)

Crystal data

$C_7H_8N_2O_2$
M_r = 152.15
Tetragonal, $I4_1/a$
a = 19.8091 (6) Å
c = 7.3503 (4) Å
V = 2884.3 (2) Å^3
Z = 16
$F(000)$ = 1280
D_x = 1.402 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9856 reflections
θ = 2.9–29.9°
μ = 0.11 mm^{-1}
T = 295 K
Block, orange
0.38 × 0.36 × 0.21 mm

Data collection

Bruker D8 Quest Eco CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.910, T_{max} = 0.999
85493 measured reflections
2296 independent reflections
1669 reflections with $I \geq 2u(I)$
R_{int} = 0.087
θ_{max} = 31.0°, θ_{min} = 3.6°
h = −30→30
k = −30→30
l = −11→11

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.075
S = 1.10
2296 reflections
172 parameters
0 restraints
0 constraints
Primary atom site location: dual
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0203P)^2 + 0.9459P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.0002
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.64835 (4)	0.50497 (4)	0.26286 (11)	0.0554 (2)
O2	0.63080 (5)	0.60946 (4)	0.21656 (11)	0.0590 (3)
N1	0.65529 (6)	0.48114 (5)	0.62579 (18)	0.0470 (2)
H1A	0.6609 (8)	0.4522 (7)	0.729 (2)	0.070 (4)
H1B	0.6776 (8)	0.4679 (7)	0.511 (2)	0.064 (4)
N2	0.62245 (4)	0.55827 (4)	0.30605 (10)	0.03423 (19)
C1	0.60055 (5)	0.52243 (4)	0.62063 (13)	0.0311 (2)

C2	0.58132 (4)	0.56176 (4)	0.46892 (11)	0.02697 (18)
C3	0.52438 (5)	0.60431 (5)	0.46971 (13)	0.0334 (2)
C4	0.48708 (6)	0.60780 (6)	0.62847 (17)	0.0454 (3)
H4	0.4425 (7)	0.6385 (8)	0.630 (2)	0.085 (5)
C5	0.50662 (6)	0.57207 (6)	0.78302 (16)	0.0496 (3)
H5	0.4765 (7)	0.5758 (8)	0.905 (2)	0.084 (5)
C6	0.56209 (6)	0.53066 (6)	0.78023 (15)	0.0430 (3)
H6	0.5777 (7)	0.5026 (7)	0.8943 (19)	0.076 (4)
C31	0.50038 (8)	0.64390 (9)	0.3083 (2)	0.0539 (3)
H31A	0.5285 (10)	0.6878 (9)	0.289 (2)	0.095 (6)
H31B	0.5014 (11)	0.6159 (9)	0.185 (2)	0.113 (7)
H31C	0.4505 (9)	0.6590 (9)	0.329 (2)	0.112 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0697 (6)	0.0555 (5)	0.0411 (4)	0.0169 (4)	0.0181 (4)	−0.0051 (4)
O2	0.0723 (6)	0.0585 (5)	0.0463 (5)	0.0022 (4)	0.0238 (4)	0.0179 (4)
N1	0.0532 (6)	0.0453 (6)	0.0425 (6)	0.0100 (5)	0.0002 (5)	0.0128 (5)
H1A	0.095 (12)	0.056 (9)	0.058 (10)	0.010 (8)	−0.011 (8)	0.020 (8)
H1B	0.085 (12)	0.062 (10)	0.046 (9)	0.022 (8)	0.003 (9)	0.004 (8)
N2	0.0370 (4)	0.0406 (5)	0.0251 (4)	−0.0009 (4)	0.0043 (3)	0.0006 (3)
C1	0.0364 (5)	0.0301 (5)	0.0269 (4)	−0.0054 (4)	0.0016 (4)	0.0023 (4)
C2	0.0302 (4)	0.0262 (4)	0.0245 (4)	−0.0032 (3)	0.0024 (3)	−0.0020 (3)
C3	0.0311 (5)	0.0328 (5)	0.0363 (5)	−0.0001 (4)	−0.0009 (4)	−0.0052 (4)
C4	0.0365 (6)	0.0483 (6)	0.0514 (7)	0.0001 (5)	0.0101 (5)	−0.0147 (5)
H4	0.068 (10)	0.088 (11)	0.099 (12)	0.016 (9)	0.010 (9)	−0.026 (9)
C5	0.0496 (7)	0.0608 (7)	0.0385 (6)	−0.0103 (6)	0.0186 (5)	−0.0122 (5)
H5	0.089 (11)	0.103 (12)	0.062 (10)	−0.008 (9)	0.025 (9)	−0.005 (9)
C6	0.0525 (7)	0.0496 (6)	0.0269 (5)	−0.0121 (5)	0.0073 (5)	0.0029 (5)
H6	0.100 (11)	0.085 (10)	0.044 (8)	−0.004 (9)	0.019 (8)	−0.001 (8)
C31	0.0511 (8)	0.0531 (8)	0.0575 (8)	0.0121 (6)	−0.0122 (7)	0.0071 (7)
H31A	0.123 (15)	0.059 (10)	0.104 (14)	0.007 (10)	−0.021 (11)	0.024 (10)
H31B	0.167 (19)	0.114 (15)	0.059 (11)	0.055 (13)	−0.029 (12)	−0.010 (11)
H31C	0.063 (11)	0.151 (16)	0.121 (15)	0.049 (11)	−0.003 (10)	0.041 (13)

Geometric parameters (Å, º)

O1—N2	1.2160 (10)	C3—C31	1.4995 (16)
O2—N2	1.2199 (10)	C4—H4	1.073 (14)
N1—H1A	0.955 (14)	C4—C5	1.3933 (18)
N1—H1B	0.987 (15)	C5—H5	1.082 (14)
N1—C1	1.3588 (14)	C5—C6	1.3714 (18)
N2—C2	1.4497 (11)	C6—H6	1.052 (15)
C1—C2	1.4125 (12)	C31—H31A	1.042 (18)
C1—C6	1.4082 (14)	C31—H31B	1.066 (17)
C2—C3	1.4081 (12)	C31—H31C	1.044 (16)
C3—C4	1.3830 (14)		

H1B—N1—H1A	117.6 (12)	H4—C4—C3	118.5 (9)
C1—N1—H1A	118.5 (9)	C5—C4—C3	120.94 (11)
C1—N1—H1B	119.6 (8)	C5—C4—H4	120.6 (9)
O2—N2—O1	121.58 (8)	H5—C5—C4	119.3 (8)
C2—N2—O1	119.61 (8)	C6—C5—C4	120.95 (11)
C2—N2—O2	118.81 (8)	C6—C5—H5	119.7 (8)
C2—C1—N1	124.70 (9)	C5—C6—C1	121.00 (11)
C6—C1—N1	118.56 (10)	H6—C6—C1	116.4 (7)
C6—C1—C2	116.61 (9)	H6—C6—C5	122.6 (7)
C1—C2—N2	118.30 (8)	H31A—C31—C3	111.8 (9)
C3—C2—N2	118.82 (8)	H31B—C31—C3	113.4 (8)
C3—C2—C1	122.88 (8)	H31B—C31—H31A	108.2 (14)
C4—C3—C2	117.48 (9)	H31C—C31—C3	109.4 (9)
C31—C3—C2	124.32 (10)	H31C—C31—H31A	106.7 (13)
C31—C3—C4	118.17 (11)	H31C—C31—H31B	107.0 (14)
O1—N2—C2—C1	35.82 (10)	N2—C2—C3—C31	3.80 (12)
O1—N2—C2—C3	−144.56 (9)	C1—C2—C3—C4	1.11 (10)
O2—N2—C2—C1	−143.35 (9)	C1—C2—C3—C31	−176.61 (11)
O2—N2—C2—C3	36.26 (10)	C1—C6—C5—C4	−0.68 (12)
N1—C1—C2—N2	0.04 (11)	C2—C1—C6—C5	3.55 (10)
N1—C1—C2—C3	−179.55 (10)	C2—C3—C4—C5	1.98 (10)
N1—C1—C6—C5	179.56 (10)	C3—C2—C1—C6	−3.81 (10)
N2—C2—C1—C6	175.79 (8)	C3—C4—C5—C6	−2.23 (13)
N2—C2—C3—C4	−178.49 (8)	C5—C4—C3—C31	179.84 (12)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*B*···O1	0.987 (15)	2.052 (15)	2.7126 (15)	122.5 (11)
N1—H1*B*···N1^{i}	0.987 (15)	2.407 (15)	3.2705 (13)	145.8 (11)
N1—H1*A*···O2^{ii}	0.955 (14)	2.285 (15)	3.2108 (15)	163.0 (13)

Symmetry codes: (i) −*y*+5/4, *x*−1/4, *z*−1/4; (ii) −*y*+5/4, *x*−1/4, *z*+3/4.